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Lowest-energy states in parity-transformation eigenspaces of $SO(N)$ spin chain

Tigran Hakobyan [a,b,*]

[a] *Yerevan State University, 1 Alex Manoogian Street, Yerevan 0025, Armenia*
[b] *Tomsk Polytechnic University, Lenin Avenue 30, 634050 Tomsk, Russia*

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Abstract

We expand the symmetry of the open finite-size $SO(N)$ symmetric spin chain to $O(N)$. We partition its space of states into the eigenspaces of the parity transformations in the flavor space, generating the subgroup $Z_2^{\times(N-1)}$. It is proven that the lowest-energy states in these eigenspaces are nondegenerate and assemble in antisymmetric tensors or pseudotensors. At the valence-bond solid point, they constitute the 2^{N-1}-fold degenerate ground state with fully broken parity-transformation symmetry.

1. Introduction

The spin-1 Heisenberg chain, in contrast to its spin-$\frac{1}{2}$ analogue, is characterized by a gap and exponentially decaying correlation as was predicted by Haldane [1]. Its low-energy behavior is perfectly modeled by Affleck–Kennedy–Lieb–Tasaki (AKLT) chain with the exact valence-bond solid (VBS) ground state [2]. The Haldane phase has many fascinating properties, like a hidden string order parameter and edge states [3]. The two spin-$\frac{1}{2}$ degrees of freedom at the edges are responsible for the fourfold near degeneracy of the open chain, which becomes exact at the AKLT point [4]. Kennedy and Tasaki (KT) explained this behavior by a spontaneous breaking

* Correspondence to: Yerevan State University, 1 Alex Manoogian Street, Yerevan 0025, Armenia.
E-mail addresses: tigran.hakobyan@ysu.am, hakob@yerphi.am.

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of a hidden $Z_2 \times Z_2$ symmetry, formed by π-rotations around the coordinate axis [5]. They define nonlocal unitary transformation mapping the string order to the usual ferromagnetic order. Recently it was observed that the Haldane phase is protected by several discrete symmetries [6,7], including the above $Z_2 \times Z_2$ [7], and is characterized by a double degeneracy of the entanglement spectrum [8].

Nowadays the spin and fermion systems with higher symmetries attract much attention due to experiments in ultracold atoms [9] (see Ref. [10] for the review). Such systems are used for the classification of symmetry protected topological phases [11] and study of the entanglement spectrum [12]. The exact VBS ground states appear for certain $SU(N)$ symmetric spin Hamiltonians [13]. The $SO(5)$ generalization of the AKLT chain has appeared in the context of ladder models [14]. The construction has been extended recently to the $SO(N)$ chain by Tu, Zhang and Xiang [15]. The authors have revealed a hidden antiferromagnetic order, which is characterized by a nonlocal string order parameter. For the finite-size open chain, the related $Z_2^{\times(N-1)}$ symmetry, which consists of the π-rotations in the coordinate planes, is broken completely for odd N and partially for even N. Nevertheless, in both cases the ground state is 2^{N-1}-fold degenerate. The parity effect in N persists also for the translationally invariant chain. In the thermodynamic limit, it is in the Haldane phase for an odd case and has a twofold degenerate ground state with broken translational symmetry for an even case. This fact is supported also by the $SO(N)$ extension [16] of the Lieb–Schultz–Mattis theorem [17].

In this article we consider the finite $SO(N)$ bilinear–biquadratic spin chain with open boundaries and site-dependent couplings. We expand the symmetry to the $O(N)$ group by the parity transformations (the coordinate reflections) in the flavor space. Then partition the entire space of states into the 2^{N-1} eigenspaces of the reflection operators, which generate another subgroup $Z_2^{\times(N-1)}$. For odd N these eigenspaces are uniquely specified the quantum numbers of the aforementioned π-rotation symmetry. For even N the additional Z_2 symmetry is needed to separate them. For wide range of parameters we prove that the lowest-level state (relative ground state) in any eigenspace is nondegenerate. It is proven that the relative ground states in all eigenspaces with k odd reflection quantum numbers form k-th order antisymmetric tensor. Herewith, the parity of k must coincide with the chain length parity. Note that the k-th and $(N-k)$-th order antisymmetric tensors differ by the additional sign under improper rotations. For example, for $k = 0, N$ both are $SO(N)$ singlets while they are, respectively, a scalar and a pseudoscalar in $O(N)$ classification. For odd N, the tensor and pseudotensor lowest-energy states alternate each other with the k growth, while for even N, both multiplets appear together. In the $SO(3)$ case, the ground state may be, at most, fourfold degenerate as was established earlier by Kennedy [18]. Using the Clebsch–Gordan decomposition of the $O(N)$ spinors, constructed by Brauer and Weyl [19], the results for general couplings are verified at the VBS point with the exactly known ground state. The parity-transformation symmetry is broken completely to 2^{N-1} degenerate vacua, associated with the relative ground states from all eigenspaces.

2. $O(N)$ symmetry and nonpositive basis

The Hamiltonian of the $SO(N)$ open spin chain with nearest-neighboring interaction in vector representation has the following form:

$$\mathcal{H} = \sum_{l=1}^{L-1} \sum_{a,b=1}^{N} \left(J_l \, T_{l+1}^{ab} T_l^{ba} \; - \; K_l \, T_{l+1}^{ba} T_l^{ba} \right). \tag{1}$$

Here the T-operators are the local projectors acting on the corresponding spin state by

$$T^{ab} = |a\rangle\langle b|.$$

The spin couplings depend on site and take positive values anywhere:

$$J_l > 0, \qquad K_l > 0. \tag{2}$$

The Hamiltonian is invariant under $SO(N)$ rotations given by the generators

$$\hat{L}^{ab} = \sum_l L_l^{ab}, \qquad L_l^{ab} = i(T_l^{ab} - T_l^{ba})$$

and can be expressed as their bilinear–biquadratic combination. Up to a nonessential constant,

$$\mathcal{H} = \sum_l \big(J_l\, \boldsymbol{L}_{l+1} \cdot \boldsymbol{L}_l + K'_l (\boldsymbol{L}_{l+1} \cdot \boldsymbol{L}_l)^2 \big), \tag{3}$$

where

$$K'_l = \tfrac{1}{N-2}(J_l - K_l),$$

and we set for the convenience

$$\boldsymbol{L}_i \cdot \boldsymbol{L}_j = \sum_{a<b} L_i^{ab} L_j^{ab}.$$

The range of new couplings is:

$$K'_l < \tfrac{1}{N-2} J_l. \tag{4}$$

It includes the integrable translationally invariant model at $K' = \frac{N-4}{(N-2)^2} J$ [20], which generalized Babujian–Takhatajan spin-1 integrable chain [21]. It also contains the model with exact VBS ground state at $K' = \frac{1}{N} J$, considered below [15,22]. Recently, its low-energy effective field theory has been studied [16].

Note that the symmetric combinations $\sum_l (T_l^{ab} + T_l^{ba})$ complement the orthogonal group to the $U(N)$. The first term in (1) just permutes the neighboring spins and possesses the unitary symmetry while the second term reduces it to the orthogonal group. In particular, it does not preserve the total number of each species,

$$\hat{N}_a = \sum_l T_l^{aa},$$

but preserves its parity. The latter corresponds to the reflection or parity transformation of the a-th flavor:

$$\hat{\sigma}_a = (-1)^{\hat{N}_a}. \tag{5}$$

The commutation with the $SO(N)$ generators is

$$\hat{\sigma}_c \hat{L}^{ab} \hat{\sigma}_c = (-1)^{\delta_{ca} + \delta_{cb}} \hat{L}^{ab}. \tag{6}$$

The reflections (5) expand $SO(N)$ symmetry of the Hamiltonian (1) to the entire orthogonal group $O(N)$, which includes also improper rotations.

Evidently, the total number of spins equals the chain length, $\sum_a N_a = L$. Therefore, the quantum numbers $\sigma_a = \pm 1$ of the flavor parity operators (5) are subjected to the rule

$$\sigma_1 \sigma_2 \dots \sigma_N = (-1)^L. \tag{7}$$

This restricts the number of independent parity transformations to $N-1$, which are reduced in this representation to the group $Z_2^{\times(N-1)}$. One can choose, for instance, the reflection operators of the first $N-1$ flavors as a set of its generators.

Let us focus first on the chains with even number of spins. In this case it can be described as a quotient of the $Z_2^{\times N}$ group, formed by independent reflections, by the Z_2 group, describing the simultaneous reflection of all flavors: $\hat{\sigma}_1 \dots \hat{\sigma}_N$. Moreover, in case of $SO(2n+1)$ symmetry, it coincides also with the group, formed by the rotations $\hat{\sigma}_a \hat{\sigma}_b$ of the planes, spanned by the a-th and b-th flavor axis, on the angle $\varphi = \pi$. Indeed, due to equation (7), any single reflection $\hat{\sigma}_a$ can be expressed in terms of the π-rotations. In particular, for the $SO(3)$ chain, they are described by the relation $\hat{\sigma}_1 = \hat{\sigma}_2 \hat{\sigma}_3$ together with two others obtained by the cyclic permutation of the indexes. For the chains with $SO(2n)$ symmetry, the relation (7) reduces the number of independent π-rotations by one, so that they form now the subgroup $Z_2^{\times(N-2)}$. An additional Z_2 reflection (one can choose, for instance, $\hat{\sigma}_1$) complements it to the entire parity-transformation group. For the odd-site chains with $SO(2n+1)$ symmetry the generators of the parity-transformation and π-rotation groups differ by sign, like in the $SO(3)$ case, where we have $\hat{\sigma}_1 = -\hat{\sigma}_2 \hat{\sigma}_3$, etc.

2.1. Nonpositive basis

The existence of basis where the off-diagonal elements of the Hamiltonian are nonpositive has a crucial significance for the proof of the nondegeneracy of the lowest-energy level in the entire space of states or the subspaces specified by good quantum numbers [23,17,24]. Such basis has no minus sign problem and can be used for Monte Carlo simulations. Various spin and fermion lattice systems possess such basis [25–28]. Usually frustration, higher-rank symmetry, or higher-order terms in the Hamiltonian create an obstacle towards it. Fortunately, it is possible to overcome them for some frustrated spin ladder systems [29,30], as well as in one-dimension for several spin systems with higher symmetries [31,34,32,33,35]. The $SU(N)$ and $SO(N)$ open spin chains in defining representation have the same nonpositive basis. It is obtained by equipping the standard basis, composed from the single spins, with the sign factor

$$\theta_{a_1 \dots a_L} = (-1)^{\{\#(i<j) | a_i > a_j\}}, \tag{8}$$

which counts the number of all inversely ordered pairs of flavors and returns its parity [32,35]:

$$\overline{|a_1 \dots a_L\rangle} = \theta_{a_1 \dots a_L} |a_1 \dots a_L\rangle. \tag{9}$$

It was defined in terms of fermions by Affleck and Lieb and used the proof of uniqueness of the ground state of $SU(2N)$ spin chain [31]. Later it was applied for fermion chains with various symmetries [26,36,37,33]. The above form of the basis has been applied for the extension of Lieb–Mattis theorem for the $SU(N)$ spin chain [32]. Recently, it has been used in Monte Carlo simulation of $SU(N)$ [38] and $SO(N)$ [35] spin chains.

The sign $\theta_{a_1 \dots a_L}$ alters under the permutation of two distinct neighboring flavors since they are the only pair which changes the order: $\theta_{\dots ab \dots} = -\theta_{\dots ba \dots}$ [32]. From the other side, it remains unchanged if two adjacent equal spins are replaced by another pair, since the inclusion of double flavors changes the amount of disordered pairs on even number: $\theta_{\dots aa \dots} = \theta_{\dots bb \dots}$ [35]. Therefore, the off-diagonal matrix elements of the Hamiltonian (1), (2) are nonpositive in the basis (9).

3. Lowest-level states in σ-subspaces

We partition the entire space of states $\mathcal{V}^L$ into 2^{N-1} subspaces, characterized by the distinct sets of the reflection quantum numbers (5) constrained by (7):

$$V^L_{\sigma_1\ldots\sigma_N} = \{\psi \,|\, \hat{\sigma}_a\psi = \sigma_a\psi\}. \tag{10}$$

We call them σ-subspaces, following a similar definition for $S^z = M$ eigenspaces [24]. The Hamiltonian (1) remains invariant in any σ-subspace, its matrix is connected there in the basis (9).

In order to verify the last claim, denote by $N_\pm$ the amount of the plus and minus indexes the subspace (10), so that $N_+ + N_- = N$. According to the restriction (7),

$$(-1)^{N_-} = (-1)^L. \tag{11}$$

Arrange all flavors with odd N_a in ascending order:

$$a_1^- < \cdots < a_{N_-}^-, \qquad \sigma_{a_i^-} = -1. \tag{12}$$

Then the Hamiltonian connects any basic state of $V^L_{\sigma_1\ldots\sigma_N}$ to the state

$$|\underbrace{1\ldots1}_{L-N_-} a_1^- \ldots a_{N_-}^-\rangle.$$

Indeed, acting by the first term in (1), one can rearrange the flavors in non-descending order. Then using the second term, one can replace any adjacent pair aa with the pair 11. The second rearrangement gives the desired state.

According to the Perron–Frobenius theorem [39], the lowest-energy state in the subspace (10) is nondegenerate and a positive superposition of the basic states (9) from the subspace (10):

$$\Omega_{\sigma_1\ldots\sigma_N} = \sum_{(-1)^{N_{a_i}}=\sigma_{a_i}} \omega_{a_1\ldots a_L}\,\overline{|a_1\ldots a_L\rangle} \tag{13}$$

with

$$\omega_{a_1\ldots a_L} > 0.$$

In order to detect the multiplet containing the relative ground state, we chose a trial state. Fill the first N_- sites by the antisymmetric combination of the flavors with odd numbers (12). The number of remaining sites of the chain is even due to (11). Divide them into neighboring pairs, fill each pair with the same flavor, then take the sum over all flavors. As a result, we arrive at the state

$$\begin{aligned}\Psi &= \sum_{s\in\mathcal{S}_{N_-}} \epsilon_{s_1\ldots s_{N_-}}\,|a^-_{s_1}\ldots a^-_{s_{N_-}}\rangle \otimes \underbrace{\psi\otimes\cdots\otimes\psi}_{k} \\ &= \sum_{s\in\mathcal{S}_{N_-}}\sum_{b_1\ldots b_k} \overline{|a^-_{s_1}\ldots a^-_{s_{N_-}} b_1b_1b_2b_2\ldots b_kb_k\rangle}\end{aligned} \tag{14}$$

with

$$\psi = \sum_b |bb\rangle \qquad \text{and} \qquad k = \tfrac{1}{2}(L - N_-).$$

The first sum performs the antisymmetrization over all flavors with $\sigma_a = -1$ using the Levi-Civita symbol. The constructed state is a positive superposition of certain states from (9), because the insertion of a neighboring particle pair with same flavor does not change the sign factor in (9). Therefore, it has a nonzero overlap with the relative ground state (13). Since the ψ state is a scalar, the trial state belongs to (N_-)-th order antisymmetric multiplet (tensor), which is described by the one-column Young tableau of the same length [40],

$$\mathbb{Y}_{N_-} = \mathbb{Y}[\underbrace{1, 1, \ldots, 1}_{N_-}]. \tag{15}$$

Remember now that the nonequivalent multiplets are mutually orthogonal. The nondegeneracy of the relative ground state implies that it must belong to a certain multiplet. The latter must be characterized by the same Young tableau (15) due to the orthogonality condition of nonequivalent multiplets.

In contrast to the Hamiltonian, the orthogonal symmetry mixes different σ-subspaces. Consider the symmetric group of permutations between different flavors, $\mathcal{S}_N \subset O(N)$. It permutes the reflection operators and the indexes of the σ-subspace:

$$s\hat{\sigma}_a s^{-1} = \hat{\sigma}_{s(a)}, \qquad sV^L_{\sigma_1\ldots\sigma_N} = V^L_{\sigma_{s(1)}\ldots\sigma_{s(N)}},$$

where $s \in \mathcal{S}_N$. Due to the symmetry, the Hamiltonian has the same spectrum on all σ-subspaces, which have the same number of negative indexes. We unify them into the $\binom{N}{N_-}$-fold degenerate subspace

$$\mathcal{V}^L_{N_-} = V^L_{\underbrace{-\cdots-}_{N_-}\underbrace{+\cdots+}_{N_+}} \oplus V^L_{\underbrace{-\cdots-}_{N_--1}+-\underbrace{+\cdots+}_{N_+-1}} \oplus \\ \cdots\cdots \oplus V^L_{\underbrace{+\cdots+}_{N_+}\underbrace{-\cdots-}_{N_-}}. \tag{16}$$

Thus, *the relative ground state in the subspace $\mathcal{V}^L_{N_-}$ is a unique (N_-)-th order antisymmetric $O(N)$ tensor. It gathers the relative ground states of all σ-subspaces from* (16).

The entire space of states represents the sum of these degenerate subspaces:

$$\mathcal{V}^L = \begin{cases} \mathcal{V}^L_N \oplus \mathcal{V}^L_{N-2} \oplus \ldots \oplus \mathcal{V}^L_0 & \text{even } N, L, \\ \mathcal{V}^L_N \oplus \mathcal{V}^L_{N-2} \oplus \ldots \oplus \mathcal{V}^L_1 & \text{odd } N, L, \\ \mathcal{V}^L_{N-1} \oplus \mathcal{V}^L_{N-3} \oplus \ldots \oplus \mathcal{V}^L_1 & \text{even } N, \text{odd } L, \\ \mathcal{V}^L_{N-1} \oplus \mathcal{V}^L_{N-3} \oplus \ldots \oplus \mathcal{V}^L_0 & \text{odd } N, \text{even } L. \end{cases} \tag{17}$$

It must be mentioned that the subspace $\mathcal{V}^L_{N_-}$ is not empty if $N_- \le L$. So we suppose in the following that the chain length is large enough, $L \ge N$.

The total ground state may be, at most, 2^{N-1}-fold degenerate combining the lowest-level multiplets from all subspaces $\mathcal{V}^L_k$ in the decomposition (17).

According to the representation theory of orthogonal algebras [40], two multiplets, described by the Young diagrams $\mathbb{Y}_{N_\pm}$, are mutually conjugate and related by the Levi-Civita symbol $\epsilon_{a_1\ldots a_N}$. The conjugate multiplets are distinguished by the sign under improper rotations, which maps tensor to pseudotensor. For example, $\mathbb{Y}_0$ is a scalar (singlet) while $\mathbb{Y}_N \sim \mathbb{Y}'_0$ is a pseudoscalar; $\mathbb{Y}_1$ is a vector while $\mathbb{Y}_{N-1} \sim \mathbb{Y}'_1$ is a pseudovector, etc. In particular, the lowest level state is a scalar in the subspace $\mathcal{V}^L_0$ and a pseudoscalar in $\mathcal{V}^L_N$. As $SO(N)$ representations, they are equivalent, and the smallest number from the set $N_\pm$ characterizes the multiplet. According to (17), the distribution on k of the lowest-level multiplets in $\mathcal{V}_k^L$ depends sharply on the parity of N. In an odd case, the tensors and pseudotensors alternate each other with the growth of k, while in an even case, both type multiplets appear together. The self-conjugate representation $\mathbb{Y}_{N/2}$ emerges only once for N being a multiple of 4.

Now turn back to the another $Z_2^{\times(N-1)}$ symmetry, formed by the π-rotations in the $\binom{N}{2}$ coordinate planes,

$$\hat{\sigma}_a\hat{\sigma}_b = e^{i\pi\hat{L}^{ab}}.$$

The σ-subspaces are the eigenspaces of its elements corresponding to the quantum numbers $\sigma_a\sigma_b$. They remain unchanged under the simultaneous change of all signs $\sigma_a \to -\sigma_a$ and, therefore, do not distinguish between conjugate representations $\mathbb{Y}_{N_\pm}$. For example, both the scalar and pseudoscalar are labeled by the plus signs. For odd N, the elements of this group parameterize uniquely the σ-subspaces, since due to the condition (11) among the two subspaces $V^L_{\sigma_1\ldots\sigma_N}$ and $V^L_{-\sigma_1\ldots-\sigma_N}$, only one exists for a given chain. In contrast, for even N, both subspaces present or absent simultaneously and belong to the subspaces $\mathcal{V}^L_{N_\mp}$ respectively. An additional Z_2 quantum number σ_1 separates them.

4. *SO*(3) case

Consider the simplest case of $SO(3)$ chain and express the bilinear–biquadratic Hamiltonian (3) through the standard spin-one operators:

$$\mathcal{H} = \sum_l \left(J_l\, \boldsymbol{S}_{l+1}\cdot\boldsymbol{S}_l + K'_l(\boldsymbol{S}_{l+1}\cdot\boldsymbol{S}_l)^2\right), \tag{18}$$

with $S_l^a = -\epsilon^{abc}L_l^{bc}$ and $K'_l < J_l$. According to the general case (16), the σ-subspaces are unified into four degenerate subspaces,

$$\begin{aligned} &\mathcal{V}_0^L = V^L_{+++}, \qquad \mathcal{V}_2^L = V^L_{+--}\oplus V^L_{-+-}\oplus V^L_{--+},\\ &\mathcal{V}_3^L = V^L_{---}, \qquad \mathcal{V}_1^L = V^L_{++-}\oplus V^L_{+-+}\oplus V^L_{-++}, \end{aligned} \tag{19}$$

so that the first or second lines happen, respectively, for the chains with even or odd lengths. Following (17), the entire space of states can be expressed in terms of them as follows:

$$\mathcal{V}^L = \begin{cases} \mathcal{V}_2^L \oplus \mathcal{V}_0^L & \text{for even } L,\\ \mathcal{V}_3^L \oplus \mathcal{V}_1^L & \text{for odd } L. \end{cases} \tag{20}$$

Applying the previously obtained results for $N = 3$ case, we conclude that *the lowest-energy states in the subspaces $\mathcal{V}_0^L$ and $\mathcal{V}_3^L$ are spin-singlets, which behave as a scalar and pseudo-scalar, correspondingly, under improper rotations. In the subspaces $\mathcal{V}_1^L$ and $\mathcal{V}_2^L$ they form spin-triplets with vector and pseudo-vector behavior. All these multiplets are nondegenerate.*

The total ground state is either a unique spin-singlet, or a unique spin-triplet, or their superposition. The first opportunity happens for $K'_l \le 0$ [25], and the last one takes place at the AKLT point $K'_l = \frac{1}{3}J_l$. So, it may be at most fourfold degenerate as was established already by Kennedy in Ref. [18]. He used another partition and another negative basis. The latter is obtained from the usual Ising basis by a nonlocal unitary shift locally equivalent to the KT transformation. Its relation with the basis (9) has been studied in detail recently [35].

5. Exact VBS case

The coupling values $K'_l = \frac{1}{N} J_l$ describe the chain with the exact 2^{N-1}-fold degenerate VBS ground state [15,22]. The couplings can be made site-dependent since the ground state minimizes apart all local interactions. The spinor representation of the orthogonal group has been used in order to obtain the explicit expression of the ground-state [14,15,22] in the matrix product form [41]. Here we adopt the construction to the open chain and show that the parity-transformation symmetry $Z_2^{\times(N-1)}$ is broken completely.

Define 2^n-dimensional gamma matrices with $n = [\frac{N}{2}]$, which generate the Clifford algebra

$$\{\Gamma^a, \Gamma^b\} = 2\delta_{ab}.$$

The spinor representation of $SO(N)$ is given by

$$L^{ab} = -\frac{i}{2}[\Gamma^a, \Gamma^b].$$

The rotation R in the flavor space induces the unitary transformation of spinors:

$$U_R \Gamma^a U_R^+ = \sum_b R_{ab} \Gamma^b. \tag{21}$$

The ground state is presented in the matrix product form [14],

$$\Omega_{\alpha\beta} \sim \sum_{a_1, a_2, \ldots, a_L} (\Gamma^{a_1} \Gamma^{a_2} \ldots \Gamma^{a_L})_{\alpha\beta} |a_1 a_2 \ldots a_L\rangle, \tag{22}$$

where α, β are 2^n-dimensional spinor indexes. The trace gives rise to the translationally invariant ground state [15]. As a result, the ground state transforms under rotations as

$$\mathbf{\Omega} \to U_R \mathbf{\Omega} U_R^+,$$

and, hence, belongs to the tensor product of the spinor representation Δ and its dual Δ^* (which are equivalent). Its Clebsch–Gordan decomposition depends on whether N is even or odd.

For $O(2n)$, it reads [19]:

$$\Delta \otimes \Delta^* = \bigoplus_{k=0}^{N} \mathbb{Y}_k = \bigoplus_{k=0}^{n-1} (\mathbb{Y}_k \oplus \mathbb{Y}'_k) \oplus \mathbb{Y}_n. \tag{23}$$

The spinor representation (21) expands to the $O(2n)$ representation by $\hat{\sigma}_a = \Gamma^a \Gamma^0$. Here

$$\Gamma^0 = \imath^n \prod_{a=1}^{N} \Gamma^a,$$

where $\imath$ is 1 or i according as n is even or odd. The multiplets $\mathbb{Y}_k$ and $\mathbb{Y}'_k$ are formed by the components of the rank k antisymmetric tensor,

$$\Omega^{b_1 \ldots b_k}_{\mathbb{Y}_k} = \mathrm{Tr}(\mathbf{\Omega} \Gamma^{[b_1} \ldots \Gamma^{b_k]}), \qquad k \le n, \tag{24}$$

$$\Omega^{b_1 \ldots b_k}_{\mathbb{Y}'_k} = \mathrm{Tr}(\mathbf{\Omega} \Gamma^0 \Gamma^{[b_1} \ldots \Gamma^{b_k]}), \qquad k < n, \tag{25}$$

where the antisymmetrization is performed over the indexes in square brackets. Since the trace of a product of odd number of gamma matrices vanishes, only the states obeying (11) survive in the sum (22). This reduces the number of nonvanishing matrix elements of $\Omega_{\alpha\beta}$ from 2^N to 2^{N-1}, as was also mentioned in Ref. [35]. The trace of a product of even number of gamma matrices is expressed in terms of the Kronecker delta products, which vanish unless their indexes coincide pairwise. Each index b_i from the trace decomposition in (24) will be paired by $\delta^{b_i a_j}$ with any index a_j from (22). The antisymmetrization eliminates the pairings between the indexes b_i. As a result, we obtain a combination of states with k distinct flavors $b_1, \ldots, b_k$ and $L-k$ flavors partitioned into the singlets ψ from (14). Therefore, the ground state

$$\Omega^{b_1\ldots b_k}_{\mathbb{Y}_k} = \mathbf{\Omega}_{\mathbb{Y}_k}$$

belongs to the subspace $\mathcal{V}^L_k$ defined in (16). Moreover, the 2^{N-1}-fold degenerate ground state splits into them in complete agreement with the decomposition (17) for even N:

$$\mathbf{\Omega} = \begin{cases} \bigoplus_{i=0}^n \mathbf{\Omega}_{\mathbb{Y}_{2i}} = \mathbf{\Omega}_{\mathbb{Y}_0} \oplus \mathbf{\Omega}_{\mathbb{Y}'_0} \oplus \mathbf{\Omega}_{\mathbb{Y}_2} \oplus \mathbf{\Omega}_{\mathbb{Y}'_2} \oplus \ldots \\ \bigoplus_{i=1}^n \mathbf{\Omega}_{\mathbb{Y}_{2i-1}} = \mathbf{\Omega}_{\mathbb{Y}_1} \oplus \mathbf{\Omega}_{\mathbb{Y}'_1} \oplus \mathbf{\Omega}_{\mathbb{Y}_3} \oplus \mathbf{\Omega}_{\mathbb{Y}'_3} \oplus \ldots, \end{cases}$$

where the first and second lines correspond, respectively, to even and odd values of L. The parity-transformation symmetry is fully broken. In contrast, the π-rotation symmetry is broken partially [15], up to the mutually conjugate multiplets. So, like for the σ-subspaces, one needs in a single Z_2 reflection in order to separate the tensors from pseudotensors and get a fully broken symmetry.

For $O(2n+1)$, the Clebsch–Gordan decomposition is [19]

$$\Delta \otimes \Delta^* = \bigoplus_{i=0}^{n} \mathbb{Y}_{2i} = \mathbb{Y}_0 \oplus \mathbb{Y}'_1 \oplus \mathbb{Y}_2 \oplus \mathbb{Y}'_3 \oplus \ldots, \tag{26}$$

where the second sum concludes with $\mathbb{Y}_n$ or $\mathbb{Y}'_n$, respectively, for even or odd n. Now Γ^0 commutes with Γ^a and is a number. A product with nonzero trace exists for any number ($\geq N$) of gamma matrices. The simultaneous flip in the sign of all flavors now is an improper rotation acting by

$$\Psi \to (-1)^L \Psi$$

on all states (7), including the ground state (22). This modifies the decomposition (26) for odd-length chains:

$$\mathbf{\Omega} = \begin{cases} \bigoplus_{i=0}^n \mathbf{\Omega}_{\mathbb{Y}_{2i}} = \mathbf{\Omega}_{\mathbb{Y}_0} \oplus \mathbf{\Omega}_{\mathbb{Y}'_1} \oplus \mathbf{\Omega}_{\mathbb{Y}_3} \oplus \ldots & \text{even } L, \\ \bigoplus_{i=0}^n \mathbf{\Omega}_{\mathbb{Y}'_{2i}} = \mathbf{\Omega}_{\mathbb{Y}'_0} \oplus \mathbf{\Omega}_{\mathbb{Y}_1} \oplus \mathbf{\Omega}_{\mathbb{Y}'_3} \oplus \ldots & \text{odd } L. \end{cases}$$

This sum corresponds to the superposition of the lowest-level multiplets inherited from the decomposition (17) for odd N. The $SO(N)$ decomposition is obtained upon the substitution $\mathbb{Y}'_k = \mathbb{Y}_k$ in both sums [22]. Like the π-rotation symmetry [15], the parity-transformation symmetry is broken completely.

The AKLT Hamiltonian corresponds to the $O(3)$ symmetric spin-1 chain (18) at $K'_l = \frac{1}{3} J_l$ [2]. The fourfold degenerate ground state splits into singlet and triplet states. For the even L, they are lowest-energy states of $\mathcal{V}^3_0$ and $\mathcal{V}^3_2$ and represented by a scalar and pseudovector, respectively. For the odd L, they are lowest-energy states of $\mathcal{V}^3_1$ and $\mathcal{V}^3_3$ and represented by a vector and pseudoscalar, respectively.

6. Conclusion

In the current article, the properties of the lowest-energy states of the $SO(N)$ bilinear-biquadratic spin chain with L spins and open boundaries are studied for wide range of couplings. We consider the reflections with respect to each flavor (parity transformations), which generate the $Z_2^{\times(N-1)}$ group, expanding the symmetry to $O(N)$. It splits the entire space of states into the 2^{N-1} subspaces $V_{\sigma_1\ldots\sigma_N}$, each characterized by the set of N reflection quantum numbers $\sigma_a = \pm$, subjected to the condition (7).

For wide range of parameters it is proven that the lowest-level state in any such σ-subspace is nondegenerate. Moreover, the lowest states from all subspaces $V_{\sigma_1\ldots\sigma_N}$ with k negative indexes form k-th order antisymmetric tensor, or $O(N)$ multiplet. In particular, the relative ground state is a scalar and pseudoscalar, respectively, in the subspaces with positive ($V_{++\ldots+}$) and negative ($V_{--\ldots-}$) signs.

As a result, the entire ground state may be, at most, 2^{N-1}-fold degenerate. The maximal degeneracy appears at the point with the exact valence-bond solid (VBS) ground state, where the $Z_2^{\times(N-1)}$ symmetry is broken completely to 2^{N-1} degenerate vacua, described by the relative ground states from all σ-subspaces. The even–odd effect both on the group rank and chain length is observed. For even N, the degenerate ground state is formed by k-th order tensor and pseudotensor multiplets. For odd N, tensor and pseudotensor multiplets alternate each other: k-th order tensor precedes the $(k+1)$-th order pseudotensor. In both cases, the parity of k has to coincide with the parity of the chain length L. In particular, the ground state of the usual spin-1 bilinear–biquadratic chain with even number of spins is the superposition of a scalar and a pseudovector, while for odd-site chain it combines a pseudoscalar and a vector.

Out of the VBS point, the degeneracy between the different multiplets is removed. However, any such multiplet still combines all lowest-level states from the σ-subspace with the same set of reflection quantum numbers σ_a. This property sheds light on the origin of the broken $Z^{\times(N-1)}$ symmetry at the VBS point.

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